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Heat kernel coefficients to the matrix Schrödinger operator

I. G. Avramidi [a) b) c)] and R. Schimming [d)]
Department of Mathematics, University of Greifswald
Jahnstr. 15a, 17489 Greifswald, Germany

The heat kernel coefficients H_k to the Schrödinger operator with a matrix potential are investigated. We present algorithms and explicit expressions for the Taylor coefficients of the H_k. Special terms are discussed, and for the one-dimensional case some improved algorithms are derived.

[a)] Alexander von Humboldt Fellow
[b)] On leave of absence from Research Institute for Physics, Rostov State University, Stachki 194, Rostov-on-Don 344104, Russia
[c)] E-mail: avramidi@math-inf.uni-greifswald.d400.de
[d)] E-mail: schimmin@math-inf.uni-greifswald.d400.de

I. INTRODUCTION

Let us consider the Laplace operator on functions over some domain $M \subseteq \mathbb{R}^n$ with Cartesian coordinates $x^a = x^1, \dots, x^n$:

$$\Delta = g^{ab}\partial_a\partial_b, \qquad \partial_a = \frac{\partial}{\partial x^a}, \tag{1.1}$$

with a constant positive definite metric $(g_{ab}) = (g^{ab})^{-1}$, and the matrix Schrödinger operator

$$L = I\Delta + U, \tag{1.2}$$

where I is the $N \times N$ unit matrix and $U = U(x)$ some $N \times N$ matrix-valued potential. We assume the potential U to be Hermitian, $U^\dagger = U$, and smooth in the domain M. If M is noncompact, it is assumed, in addition, that $U(x)$ decreases sufficiently rapidly at infinity.

It is well known that L is an elliptic and self-adjoint operator with a real spectrum bounded from above on a Hilbert space of functions over M with some suitable boundary conditions. In the case of a periodic potential the boundary conditions can be replaced by periodicity conditions, and in the case of a noncompact domain they take the form of some asymptotic conditions at infinity, requiring sufficiently fast decrease.

This implies that for any $t > 0$ the operator $K(t) = \exp(tL)$ is well defined. Its kernel $K(x, x'; t)$, often referred to as the heat kernel, is the fundamental solution of the heat equation

$$(I\partial_t - L)K = 0; \tag{1.3}$$

it satisfies a singular initial condition

$$K(x, x'; +0) = (\det g_{ab})^{-1/2}\delta(x - x')I, \tag{1.4}$$

where $\delta(x)$ denotes the Dirac delta-distribution. It is well known that when the points x and x' do not lie on the boundary, there holds an asymptotic expansion as $t \to +0$ near the diagonal $x \approx x'$ of the form

$$K(x, x'; t) \sim (4\pi t)^{-n/2} \exp\left\{-\frac{1}{4t}|x - x'|^2\right\} \sum_{k=0}^{\infty} t^k H_k(x, x'), \tag{1.5}$$

where $|x| = g_{ab}x^a x^b$. From (1.3) and (1.5) it follows that the sequence of the coefficients H_k is characterized by the differential-recursion relations

$$(D + k)\, H_k = L H_{k-1}, \qquad \text{for } k \geq 1, \tag{1.6}$$

where we abbreviate

$$D = (x - x')^a \partial_a, \tag{1.7}$$

together with the initial condition

$$H_0 = I. \tag{1.8}$$

The analysis of the heat kernel, or Hadamard, coefficients $H_k = H_k(x, x'), (k = 0, 1, 2 \ldots)$, introduced by (1.6)-(1.8) is the subject of the present paper. Their role goes far beyond the heat kernel. They can be introduced for any linear second order differential operator with a Laplace-like principal part (cf. e.g.[1−5]). The sequence (H_k) turns out to have diverse mathematical and physical applications: spectral geometry, Hadamard's elementary solution, Huygens' principle, statistical physics, determinants of elliptic operators, anomalies, Korteweg-de Vries hierarchy of soliton equations etc.

In the present paper we assume the metric (g_{ab}) to be Euclidean, i.e. positive definite, and the operator L to be elliptic for the sake of simplicity. The formal results hold for a pseudo-Euclidean metric of any signature and hyperbolic (normally hyperbolic or ultrahyperbolic) operators too.

Our paper is organized as follows. In Sects. II and III we obtain explicit formulas for the Taylor coefficients $[d^p H_k](p = 0, 1, 2, \ldots)$ of $H_k(x, x')$, where x is the variable point and x' is the origin. We analyse these quantities and determine some special terms and a 'common denominator' (see below). In Sect. IV we consider the one-dimensional case and derive a simplified algorithm for the diagonal values $[H_k]$ of the H_k via a matrix Riccati equation. Then we generalize the so-called 'Lenard recursion' from the scalar case to the matrix one. The new recursion is formally non-local, but can be effectively done in the space of differential polynomials in U. It leads to a proposal of some matrix Korteweg-de Vries hierarchy for $U = U(x, \tau)$.

It is not possible to quote all the literature on the heat kernel approach. Let us mention papers which deal with the matrix case[6−12]. The methods applied there differ from ours.

II. THE HEAT KERNEL COEFFICIENTS

For a smooth potential $U = U(x)$ the coefficients $H_k(x, x')$ are known to be smooth near the diagonal $x = x'$. Thus, to study the sequence (H_k) we use the Taylor expansion with respect to the variable x at the origin x' taken as an asymptotic series as $x \to x'$:

$$H_k(x, x') \simeq \sum_{p=0}^{\infty} \frac{1}{p!} (x - x')^{a_1} \cdots (x - x')^{a_p} [\partial_{a_1} \cdots \partial_{a_p} H_k]. \tag{2.1}$$

Here and in the following the square brackets [ ] denote the diagonal value of a two-point quantity $H = H(x, x')$:

$$[H] = [H](x) := H(x, x). \tag{2.2}$$

The coefficients of the Taylor expansion can be arranged to matrix-valued symmetric differential forms (or covariant tensors), shortly p-forms,. The symmetric product $\vee$ of two such forms $A_{(p)}$ and $B_{(q)}$ is defined as

$$A_{(p)} \vee B_{(q)} = A_{(a_1 \cdots a_p} B_{b_1 \cdots b_q)} dx^{a_1} \otimes \cdots \otimes dx^{a_p} \otimes dx^{b_1} \otimes \cdots \otimes dx^{b_q}, \tag{2.3}$$

where the parentheses mean symmetrization over all indices included. The symmetric differential

$$d : A_{(p)} \to A_{(p+1)} \tag{2.4}$$

on these forms is defined by

$$dA_{(p)} = \partial_{(a_1} A_{a_2\cdots a_{p+1})} dx^{a_1} \otimes \cdots \otimes dx^{a_{p+1}}. \tag{2.5}$$

Using these notations, we have

$$[d^p H_k] = [\partial_{a_1} \cdots \partial_{a_p} H_k] dx^{a_1} \otimes \cdots \otimes dx^{a_p}. \tag{2.6}$$

Further, we define some trace operation

$$g^{-1} : A_{(p)} \to A_{(p-2)} \tag{2.7}$$

by

$$\begin{aligned} &g^{-1} A_{(0)} = 0, \qquad g^{-1} A_{(1)} = 0, \\ &g^{-1} A_{(p)} = g^{a_1 a_2} A_{(a_1 a_2 a_3 \cdots a_p)} dx^{a_3} \otimes \cdots \otimes dx^{a_p}, \qquad \text{for } p \geq 2. \end{aligned} \tag{2.8}$$

The Laplacian on symmetric forms

$$\Delta := g^{-1} d^2 : \ A_{(p)} \to A_{(p)} \tag{2.9}$$

generalizes the usual Laplacian (1.1) on functions, i.e. $0-$forms.

Let us now apply d^p to (1.6) and then restrict to the diagonal $x = x'$. Taking into account the commutation relation

$$[d^p, D] = p d^p, \tag{2.10}$$

we obtain the purely algebraic recursion system

$$(p+k)[d^p H_k] = g^{-1}[d^{p+2} H_{k-1}] + \sum_{q=0}^{p} \binom{p}{q} U_{(p-q)} \vee [d^q H_{k-1}], \qquad \text{for } k \geq 1, \qquad p \geq 0 \tag{2.11}$$

where $U_{(p)} = d^p U$, with the initial conditions

$$[H_0] = I, \qquad [d^p H_0] = 0 \qquad \text{for } p \geq 1. \tag{2.12}$$

An explicit non-recursive solution of (2.11), (2.12) can be presented by means of the following symbolism. Let us define linear operators $M_q, (q = -2, -1, 0, 1, \ldots)$ on matrix-valued symmetric forms $A_{(p)}$ according to

$$M_{-2} A_{(p)} := g^{-1} A_{(p)}, \qquad M_{-1} A_{(p)} := 0, \tag{2.13}$$

$$M_q A_{(p)} := \binom{p+q}{q} U_{(q)} \vee A_{(p)}, \qquad \text{for } q \geq 0. \tag{2.14}$$

Then the system (2.11) can be rewritten in a short-hand notation:

$$[d^p H_k] = \sum_{q=0}^{p+2} \frac{1}{p+k} M_{p-q} [d^q H_{k-1}]. \tag{2.15}$$

By applying mathematical induction to this recursion system we obtain the following.

Theorem 2.1. *There holds for $k \geq 1, p \geq 0$*

$$[d^p H_k] = \sum_{q_2,\dots,q_k} \left(\prod_{r=1}^{k} \frac{1}{(q_r + k - r + 1)} M_{q_r - q_{r+1}} \right) I, \tag{2.16}$$

where the sum runs over the integers $q_2, q_3, \dots, q_k$ so that

$$0 \leq q_{r+1} \leq q_r + 2, \qquad \text{for } r = 1, 2, \dots, k-1,$$

and

$$q_1 = p, \qquad q_{k+1} = 0.$$

This result can also be obtained, as a special case, from the general explicit formula for the heat kernel coefficients for any second-order elliptic operator of Laplace type obtained by one of the authors (I.G.A.) in[5].

The formula (2.16) is not well suited to recognize special polynomial constituents of $[d^p H_k]$. To do this, we decompose $[d^p H_k]$ into its homogeneous parts of *degree d* with respect to U:

$$[d^p H_k] = \sum_{d=1}^{k} H^{(p)}_{k,d}. \tag{2.17}$$

The system (2.11) decomposes in an easy way into homogeneous parts too. Thereby the linear and the highest degree parts decouple from the whole system:

$$(p+k) H^{(p)}_{k,1} = g^{-1} H^{(p+2)}_{k-1,1}, \tag{2.18}$$

$$(p+k) H^{(p)}_{k,k} = \sum_{q=0}^{p} \binom{p}{q} U_{(p-q)} \vee H^{(q)}_{k-1,k-1}. \tag{2.19}$$

The initial values are given by

$$(p+1) H^{(p)}_{1,1} = U_{(p)}. \tag{2.20}$$

Mathematical induction gives the following.

Theorem 2.2. *The linear part $H^{(p)}_{k,1}$ of $[d^p H_k]$ equals*

$$H^{(p)}_{k,1} = \frac{(p+k-1)!}{(p+2k-1)!} d^p \Delta^{k-1} U, \tag{2.21}$$

while the highest degree part of $H^{(p)}_{k,k}$ *of* $[d^p H_k]$ *is*

$$H^{(p)}_{k,k} = \sum_{q_2,\cdots,q_k} \bigvee_{r=1}^{k} \frac{1}{q_r + k - r + 1} \binom{q_r}{q_{r+1}} U_{(q_r - q_{r+1})}, \tag{2.22}$$

where the sum runs over the integers $q_2, q_3, \cdots q_k$, *so that*

$$0 \le q_{r+1} \le q_r \qquad \text{for} \ \ r = 1, 2, \dots, k-1$$

$$q_1 = p, \qquad q_{k+1} = 0.$$

Let us call a number-theoretical function $d(p,k)$ a *common denominator* to the system of differential polynomials $[d^p H_k]$ if all the modified polynomials in $U, U_{(1)}, U_{(2)}, \dots$

$$\bar{H}^{(p)}_k := d(p,k)[d^p H_k] \tag{2.23}$$

have integer coefficients.

Proposition 2.3. *A common denominator in the aforesaid sense is given by*

$$d(p,k) = \frac{1}{p!} \prod_{j=0}^{l-1} \frac{(p + 2k - 2j - 1)!}{(2j)!}, \qquad \text{for even } k = 2l, \tag{2.24}$$

and

$$d(p,k) = \frac{p+k}{p!} \prod_{j=0}^{l-1} \frac{(p + 2k - 2j - 1)!}{(2j)!}, \qquad \text{for odd } k = 2l - 1, \tag{2.25}$$

Proof. Substituting

$$[d^p H_k] = \frac{1}{d(p,k)} \bar{H}^{(p)}_k \tag{2.26}$$

into (2.11) we get the recursion system for the $\bar{H}^{(p)}_k$

$$\bar{H}^{(p)}_k = \frac{d(p,k)}{(p+k)d(p+2,k-1)} g^{-1} \bar{H}^{(p+2)}_{k-1} + \sum_{q=0}^{p} \binom{p}{q} \frac{d(p,k)}{(p+k)d(q,k-1)} U_{(p-q)} \vee \bar{H}^{(q)}_{k-1}, \tag{2.27}$$

for $k \ge 1, p \ge 0$. One can show that the coefficients of this system are integer, which proves the theorem.

To find the *least* common denominator remains an open problem. Fulling[13] found the expressions (2.24), (2.25) except for the factor $1/p!$. It is obvious, that this factor does not matter for $p = 0$.

III. THE DIFFERENTIAL POLYNOMIALS $[H_k]$

Let us analyse more closely the structure of the differential polynomials $[H_k]$. The common denominator for the system $[H_k], (k = 1, 2, \cdots)$ reads

$$d(0,k) = \prod_{j=0}^{[(k-1)/2]} \frac{(2k-2j-1)!}{(2j)!}. \tag{3.1}$$

The extremal terms are given by

$$[H_k] = \frac{(k-1)!}{(2k-1)!}\Delta^{k-1}U + \cdots + \frac{1}{k!}U^k, \qquad \text{for } k \geq 1, \tag{3.2}$$

where the points indicate terms of a degree higher than 1 and less than k. The sequence begins with

$$\begin{aligned} [H_1] &= U, \\ [H_2] &= \frac{1}{6}\left(\Delta U + 3U^2\right), \\ [H_3] &= \frac{1}{60}\left\{\Delta^2 U + 5\left[U(\Delta U) + (\Delta U)U + g^{-1}(dU \vee dU)\right] + 10U^3\right\}. \end{aligned} \tag{3.3}$$

Using the identity

$$2g^{-1}(dW_1 \vee dW_2) = \Delta(W_1 W_2) - (\Delta W_1)W_2 - W_1(\Delta W_2), \tag{3.4}$$

whith W_1, W_2 being 0-forms , one can eliminate the operator g^{-1} here:

$$[H_3] = \frac{1}{120}\left\{2\Delta^2 U + 5U(\Delta U) + 5(\Delta U)U + 5\Delta(U^2) + 20U^3\right\}. \tag{3.5}$$

Let us call a monomial or differential polynomial *simple* if it is solely composed from U and Δ (but not from d and g^{-1}), and the total number of symbols U and Δ in a simple monomial the *weight* w. It is obvious that a simple monomial is always a 0-form and that the number of symbols U in it equals its degree.

Theorem 3.1. *There are exactly*

$$C(w,d) = \frac{1}{w}\binom{w}{d}\binom{w}{d-1} \tag{3.6}$$

simple monomials of degree d and weight w.

Proof. A simple monomial W reads $W = U^w$ or

$$W = U^{d_0}(\Delta W_1)W_2, \tag{3.7}$$

where U^{d_0} and W_2 may be empty, while W_1 is not. Since the decomposition is unique, the number $C(w,d)$ of monomials W follows from the numbers $C(w_1,d_1), C(w_2,d_2)$ of W_1, W_2 respectively. Thus,

$$C(w,d) = \sum_{d_0=0}^{w-1} \sum_{d_1,d_2;w_1,w_2} C(w_1,d_1)C(w_2,d_2) \tag{3.8}$$

for $d < w$, where the inner sum runs over integers w_1, w_2, d_1, d_2 so that

$$w_1 \geq d_1 \geq 1, \qquad w_2 \geq d_2 \geq 0, \qquad w_1 + w_2 = w - d_0 - 1, \qquad d_1 + d_2 = d - d_0.$$

The recursion formula (3.8) can be translated into a quadratic equation

$$xyF^2 + (x+y-1)F + 1 = 0 \tag{3.9}$$

for the generating function

$$F = F(x,y) = \sum_{w=1}^{\infty}\sum_{d=1}^{w} C(w,d)x^{d-1}y^{w-d}, \tag{3.10}$$

with the initial condition

$$F(0,0) = 1. \tag{3.11}$$

Further, using

$$(1+\sqrt{1-4z})^{-1} = \frac{1}{4}\sum_{w=0}^{\infty} \frac{1}{w+1}\binom{2w}{w} z^w \tag{3.12}$$

we expand the solution of the equation (3.9)

$$F(x,y) = 2\left(1 - x - y + \sqrt{(1-x-y)^2 - 4xy}\right)^{-1} \tag{3.13}$$

in the power series (3.10) and prove that (3.6) is correct.

B. Fiedler[14] derived special cases of theorem 3.1, namely for $w = 2$ and $w = 3$, by combinatorial arguments.

Now, let us try to eliminate g^{-1} from the differential polynomials by means of the identities like (3.4). Making use of

$$2g^{-1}(dW_1 \vee W_2 \vee dW_3) = \Delta(W_1W_2W_3) - (\Delta(W_1W_2))W_3 - W_1\Delta(W_2W_3) + W_1(\Delta W_2)W_3. \tag{3.14}$$

where W_i are 0-forms, we easily get a simple form for $[H_4]$:

$$[H_4] = \frac{1}{120}\Bigg\{\frac{1}{7}\Delta^3 U + \frac{1}{3}\left[\Delta^2 U^2 + (\Delta^2 U)U + U\Delta^2 U + (\Delta U)^2 + \Delta((\Delta U)U) + \Delta(U(\Delta U))\right]$$
$$+ \Delta(U^3) + (\Delta(U^2))U + U\Delta(U^2) + (\Delta U)U^2 + U^2\Delta U + U(\Delta U)U + 5U^4\Bigg\}. \tag{3.15}$$

However, it is impossible to do this for higher polynomials $[H_k], k \geq 5$, because of terms like

$$g^{ac}g^{bd}(\partial_a W_1)(\partial_b W_2)(\partial_c W_3)(\partial_d W_4).$$

One of the authors (R.Sch.) has calculated $[H_1], \ldots, [H_4]$ in simple form for the matrix Schrödinger operator in the early paper[15]. Later T. Osborn et al.[8] obtained the result in a "non-simple" form. The other author (I.G.A.) calculated the coefficients $[H_1], \ldots, [H_4]$ in the general case, that means for every Laplace-type operator, in[16,17,5].

IY. THE ONE-DIMENSIONAL CASE

Let us discuss more detailed the one-dimensional Schrödinger operator

$$L = d^2 + U, \tag{4.1}$$

where now $d = d/dx$ and n=1. In this case the recursion system (2.11), (2.12) reduces to

$$(p+k)[d^p H_k] = [d^{p+2} H_{k-1}] + \sum_{q=0}^{p} \binom{p}{q} U_{p-q} [d^q H_{k-q}] \qquad \text{for } k \geq 1, p \geq 0 \tag{4.2}$$

$$[H_0] = I, \qquad [d^p H_0] = 0, \qquad \text{for } p \geq 1.$$

The explicit solution (2.16) of this system can be rewritten now in a better form.

Theorem 4.1. *There holds for $k \geq 2, p \geq 0$*

$$[d^p H_k] = \sum_{q_2, \cdots, q_k} \prod_{r=1}^{k} \frac{c(q_r, q_{r+1})}{q_r + k - r + 1} U_{q_r - q_{r+1}}, \tag{4.3}$$

where

$$U_{-2} := I, \qquad U_{-1} := 0, \qquad U_p := U_p = d^p U \qquad \text{for } p \geq 0, \tag{4.4}$$

$$c(p,q) := \binom{p}{q} + \delta_q^{p+2}, \tag{4.5}$$

and the sum runs over the integers $q_2, q_3, \cdots, q_k$ so that

$$0 \leq q_{r+1} \leq q_r + 2 \qquad \text{for } r = 1, 2, \cdots, k-1,$$

$$q_1 = p, \qquad q_{k+1} = 0.$$

A proof has been given by R.Sch. in[18] for the scalar case ($N = 1$). Inspection shows that the arguments of[18] do not depend on the number N of components and are valid for the matrix case too. Fulling[13] found that formula (4.3) is well suited for calculating the quantities $[d^p H_k]$ by means of computer algebra. This theorem also follows, as a rather

special case, from the results obtained by I.G.A. in[5], where a general explicit formula for the heat kernel coefficients to any second-order elliptic operator of Laplace type is obtained.

From Theorem 4.1. it follows that the quantity $[d^p H_k]$ for $k \geq 1, p \geq 0$ can be brought into the form

$$[d^p H_k] = \sum_{d=1}^{k} \sum_{r_1,\ldots,r_d \geq 0} a(r_1, r_2, \ldots, r_d) U_{r_1} U_{r_2} \cdots U_{r_d}, \tag{4.6}$$

where $a(r_1, r_2, \ldots, r_d)$ are some positive coefficients and the inner sum runs over the integers $r_1, r_2 \ldots, r_d$ so that

$$r_1 + r_2 + \cdots + r_d = p + 2(k - d).$$

There is a one-to-one correspondence between the ordered partitions $(r_1 + 1, r_2 + 1, \cdots, r_d + 1)$ of $s = \sum_{i=1}^{d}(r_i + 1) = p + 2k - d$ into d numbers and the monomials $U_{r_1} U_{r_2} \cdots U_{r_d}$. Since there are exactly $\binom{s-1}{d-1}$ such partitions, the total number of monomials, i.e. the total number of the terms in the sum (4.6) equals

$$\sum_{d=1}^{k} \binom{p + 2k - d - 1}{d - 1}. \tag{4.7}$$

The formula (4.3) is explicit, i.e. non-recursive, but somewhat complicated because each coefficient $c(q_r, q_{r+1})$ comprises the two cases $q_{r+1} \leq q_r$ and $q_{r+1} = q_r + 2$. As an alternative, we offer a recursion for the sequence $[H_k], (k = 0, 1, 2, \ldots)$ which is by far more effective than the double recursion (4.2) for the double sequence $[d^p H_k], (p, k = 0, 1, 2, \ldots)$.

Theorem 4.2. *Let the differential polynomials $Z_k, (k = 1, 2, \ldots)$ in $U = U(x)$ be recursively defined by*

$$Z_{k+1} = dZ_k + \sum_{m=1}^{k-1} Z_m Z_{k-m} \tag{4.8}$$

$$Z_1 = U. \tag{4.9}$$

Then the quantities

$$G_k := \frac{(2k)!}{2k!}[H_k] \tag{4.10}$$

are determined by the recursion

$$G_k = 2 \sum_{m=1}^{k} Z_{2m-1} G_{k-m}, \qquad \text{for } k \geq 1, \tag{4.11}$$

together with the initial condition

$$G_0 = \frac{1}{2} I. \tag{4.12}$$

Proof. Let us start with the heat kernel $K(x, x'; t)$ to L. Its Laplace transform

$$G(x, x'; \lambda) = \int_0^\infty dt \exp(-t\lambda) K(x, x'; t). \tag{4.13}$$

is the resolvent kernel to L, i.e. the fundamental solution of $L - \lambda I$, which means

$$(d^2 + U(x) - \lambda I)G(x, x'; \lambda) = -\delta(x - x')I. \tag{4.14}$$

The resolvent kernel is continuous but not differentiable at $x = x'$. Near the diagonal, $x \approx x'$, it has the form

$$G(x, x'; \lambda) = [G(\lambda)](x') - \frac{1}{2}|x - x'| + (x - x')F(x'; \lambda) + O((x - x')^2), \tag{4.15}$$

where $[G(\lambda)](x) := G(x, x; \lambda)$, so that

$$dG(x, x'; \lambda) = -\frac{1}{2}\text{sign}(x - x') + F(x'; \lambda) + O(x - x'), \tag{4.16}$$

where $|x|$ is the absolute value of x, $\text{sign}(x)$ denotes the sign of x and $F(x'; \lambda)$ is some matrix that does not depend on x. For sufficiently large $\text{Re}\lambda$ and $x \approx x'$ the resolvent kernel is known to be invertible, so that one can present the derivative of the resolvent in the form

$$dG(x, x'; \lambda) := Z(x, x'; \lambda)G(x, x'; \lambda). \tag{4.17}$$

Then from (4.16), (4.17) we conclude that $Z = Z(x, x'; \lambda)$ is discontinuous with a jump at $x = x'$ that determines the resolvent kernel on the diagonal:

$$\{Z(x' + 0, x'; \lambda) - Z(x' - 0, x'; \lambda)\}[G(\lambda)](x') = -I. \tag{4.18}$$

Moreover, the equation (4.14) for $x \neq x'$ becomes equivalent to the Riccati equation for Z

$$dZ(x, x'; \lambda) + Z^2(x, x'; \lambda) + U(x) - \lambda I = 0. \tag{4.19}$$

Let us look for a solution of this equation in the form of an asymptotic expansion as $\text{Re}\,\lambda \to \infty$, $|\text{arg}\lambda| < \pi$. Using the asymptotic expansion of the heat kernel (1.5) and (4.13) we obtain

$$Z(x, x'; \lambda) \sim X(x; \lambda) + \text{sign}(x - x')Y(x; \lambda), \tag{4.20}$$

where the formal power series

$$X(x; \lambda) = \sum_{k=0}^{\infty} (4\lambda)^{-k} Z_{2k}(x), \tag{4.21}$$

$$Y(x; \lambda) = \sum_{k=0}^{\infty} (4\lambda)^{-k+1/2} Z_{2k-1}(x), \tag{4.22}$$

are composed of the quantities $Z_k(x)$ defined above. Namely, substituting the expansion into the Riccati equation (4.19), we find that $Z_{-1} = I, Z_0 = 0$ and $Z_k(x), (k = 1, 2, \dots)$, are just the differential polynomials in $U(x)$ determined by the recursion system (4.8), (4.9).

Therefore, the asymptotic expansion of $Z(x, x'; \lambda)$ is purely local but discontinuous at $x = x'$. From (4.20) it is clear that the jump of $Z(x, x'; \lambda)$ at $x = x'$ equals just $Y(x; \lambda)$, so that (4.18) takes the form

$$2Y(x;\lambda)[G(\lambda)](x) = I \tag{4.23}$$

Using (4.13) and the asymptotic expansion of the heat kernel on the diagonal as $t \to +0$

$$[K(t)] \sim (4\pi)^{-1/2} \sum_{k=0}^{\infty} t^{k-1/2} [H_k], \tag{4.24}$$

we easily get the corresponding asymptotic expansion of the resolvent on the diagonal as $\lambda \to \infty$:

$$[G(\lambda)] \sim 2 \sum_{k=0}^{\infty} (4\lambda)^{-k-1/2} G_k, \tag{4.25}$$

where

$$G_k := \frac{(2k)!}{2k!} [H_k]. \tag{4.26}$$

Therefrom, using (4.22) and (4.23), we find that the coefficients G_k are determined by the recursion system (4.11), which proves the theorem.

The result of the Theorem 4.2. can be also obtained from the results of the paper of Fulling[7], who uses a different method and notation.

One can explicitly find the linear and quadratic parts of the differential polynomials Z_k and G_k.

Theorem 4.3. *There holds for $k \geq 3$*

$$Z_k = U_{k-1} + \sum_{p=0}^{k-3} \left\{ \binom{k-1}{p+1} - 1 \right\} U_p U_{k-3-p} + \cdots, \tag{4.27}$$

where the points indicate terms of degrees higher than two.

Proof. The linear $Z_{k,1}$ and quadratic $Z_{k,2}$ parts of Z_k satisfy the recursion systems

$$Z_{k+1,1} = dZ_{k,1}, \qquad Z_{1,1} = U, \tag{4.28}$$

$$Z_{k+1,2} = dZ_{k,2} + \sum_{m=1}^{k-1} Z_{m,1} Z_{k-m,1}, \qquad Z_{3,2} = U_2. \tag{4.29}$$

Mathematical induction gives (4.27).

Conclusion 4.4. *There holds for $k \geq 2$*

$$G_k = U_{2k-2} + \sum_{p=0}^{2k-4} \left\{ \binom{2k-2}{p+1} + (-1)^p \right\} U_p U_{2k-4-p} + \cdots + \frac{1}{2} \binom{2k}{k} U^k, \tag{4.30}$$

where the points indicate terms of degrees higher than two and less than k.

Proof. The linear $G_{k,1}$ and the highest degree $G_{k,k}$ parts of G_k follow immediately from (4.11). Therefrom we have also for the quadratic part $G_{k,2}$

$$G_{k,2} = 2 \sum_{m=1}^{k-1} Z_{2m-1,1} G_{k-m,1} + Z_{2k-1,2}. \tag{4.31}$$

Explicit calculation gives the result.

Note that in the scalar case $G_{k,2}$ had been found by means of a completely different method by Gilkey[19].

Let us now derive another recursion system for the differential polynomials G_k. Let in the following the square and the curly brackets denote the commutator and anticommutator of matrices respectively.

Theorem 4.5. *There exist unique differential polynomials*

$$W_k =: d^{-1}[G_k, U], \tag{4.32}$$

to the sequence $G_k (k = 1, 2, \ldots)$ of differential polynomials in U defined by (4.11), (4.8), (4.9), so that

$$[G_k, U] = dW_k, \tag{4.33}$$

and the G_k satisfy the differential-recursion system

$$dG_{k+1} = d^3 G_k + \{Ud + dU, G_k\} + [d^{-1}[G_k, U], U]. \tag{4.34}$$

Proof. Let us consider once more the equation for the resolvent kernel

$$d^2 G(x, x'; \lambda) + (U(x) - \lambda I) G(x, x'; \lambda) = -\delta(x - x') I. \tag{4.35}$$

As assumed from the beginning, the matrix-valued potential is Hermitian, $U^\dagger = U$, so that the Schrödinger operator is self-adjoint, $L^\dagger = L$, and the resolvent satisfies the symmetry condition

$$G^\dagger(x, x'; \lambda) = G(x', x; \lambda). \tag{4.36}$$

Using this property and interchanging the variables x and x' we get another differential equation for G:

$$d'^2 G(x, x'; \lambda) + G(x, x'; \lambda)(U(x) - \lambda I) = -\delta(x - x') I. \tag{4.37}$$

where $d' = d/dx'$.

The difference of (4.35) and (4.37) reads

$$(d + d')(d - d') G(x, x'; \lambda) = G(x, x'; \lambda) U(x') - U(x) G(x, x'; \lambda). \tag{4.38}$$

For every smooth two-point function $H(x, x')$ there holds

$$[(d + d')H] = d[H]. \tag{4.39}$$

Using this rule and restricting (4.38) to the diagonal $x = x'$, we get

$$[[G], U] = d[(d - d')G], \tag{4.40}$$

or put in another way

$$d^{-1}[[G], U] = [(d - d')G]. \tag{4.41}$$

Both $[G(\lambda)]$ and $W(\lambda) := [(d - d')G(\lambda)]$ admit asymptotic expansions in powers of $\lambda^{-1/2}$, where the coefficients G_k and W_k respectively are differential polynomials in U. Hence there are unique differential polynomials W_k such that

$$dW_k = [G_k, U]. \tag{4.42}$$

Now, let us apply the operators $(d + 3d')$ and $(d' + 3d)$ to the equations (4.35) and (4.37) respectively and then take the sum. Restricting to the diagonal the result

$$\begin{aligned}
&(d + d')^3 G(x, x'; \lambda) - 4\lambda(d + d')G(x, x'; \lambda)\\
&+ (dU(x))G(x, x'; \lambda) + G(x, x'; \lambda)d'U(x')\\
&+ 2U(x)(d + d')G(x, x'; \lambda) + 2((d + d')G(x, x'; \lambda))U(x')\\
&- U(x)(d - d')G(x, x'; \lambda) + ((d - d')G(x, x'; \lambda))U(x') = 0,
\end{aligned} \tag{4.43}$$

and using (4.39), we obtain

$$d^3[G] - 4\lambda d[G] + 2\{U, d[G]\} + \{dU, [G]\} + [d^{-1}[[G], U], U] = 0 \tag{4.44}$$

Substitution of the asymptotic expansion of the resolvent kernel on the diagonal (4.25) proves that the quantities G_k satisfy the recursion system (4.34).

The formula (4.34) has been found first by Olmedilla et al.[10], (see also the recent paper of Bilal[11]). In the scalar case, when all commutators vanish, it is known under the name 'Lenard recursion'. As a matter of fact, Burchnall and Chaundy[20] discovered the sequence (G_k) and the scalar 'Lenard recursion' already in the twenties.

Let us write (4.34) in the form

$$dG_{k+1} = BG_k \tag{4.45}$$

where the linear operator B is defined by

$$BH := d^3H + 2\{U, dH\} + \{dU, H\} + [d^{-1}[H, U], U] \tag{4.46}$$

Since the operator d is formally anti-selfadjoint, $d^\dagger = -d$, so is B:

$$B^\dagger = -B. \tag{4.47}$$

In the scalar case all the commutators vanish and B becomes a differential operator

$$B = d^3 + 2Ud + 2dU, \tag{4.48}$$

where the factor U means multiplication by U. The recursion system (4.45) can be formally solved:

$$G_k = \frac{1}{2}(d^{-1}B)^k \cdot I. \tag{4.49}$$

Thereby, the action of the positive powers of the operator B on the identity matrix is well-defined and produces the differential polynomials G_k.

A special motivation for the study of the one-dimensional Schrödinger equation is its relation to the Korteweg-de Vries (KdV) hierarchy. If one assumes a one-parameter dependence of the potential $U = U(x,\tau)$, then the differential polynomials $G_k = G_k[U](k = 1, 2, \ldots)$ constructed above constitute the KdV hierarchy in the scalar case:

$$\frac{\partial}{\partial \tau}U = \frac{\partial}{\partial x}G_k[U]. \tag{4.50}$$

For $k = 1$ a linear differential equation emerges, for $k = 2$ we have the KdV equation itself, for $k \geq 2$ the equation (4.50) is called a higher KdV equation. Moreover, it is known that (in the scalar case again) the quantities G_k as well as the Z_k are conserved densities to the KdV equation. Several papers discuss a matrix KdV equation[12,21,22]

$$\frac{\partial}{\partial \tau}U = \frac{\partial}{\partial x}G_2 = (\partial_x)^3 U + 3(\partial_x U)U + 3U(\partial_x U). \tag{4.51}$$

In particular, Olmedilla[12] proved that (4.51) is solitonic in the sense that the inverse scattering method works for (4.51). One might guess a solitonic character for the whole matrix KdV hierarchy (4.50) ($k = 2, 3, \ldots$).

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